

# Ultrahigh Dimensional Feature Selection via Kernel Canonical Correlation Analysis

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## Abstract

High-dimensional variable selection is important in many scientific fields, such as genomics. In this paper, we develop a Sure Independence feature Screening procedure based on Kernel Canonical Correlation Analysis (KCCA-SIS, for short). No model assumption is needed between response and predictors to apply KCCA-SIS and it can be used in ultrahigh dimensional data analysis. Compared to the original SIS (Fan and Lv, 2008), KCCA-SIS can handle nonlinear dependencies among variables. Compared to Distance Correlation-SIS (Li et al., 2012), KCCA-SIS is scale free, distribution free and has better approximation results based on the universal characteristic of Gaussian Kernel (Micchelli et al., 2006). KCCA-SIS encompasses SIS and DC-SIS in the sense that SIS and DC-SIS correspond to specific kernel choices under KCCA-SIS. Compared to sup-HSIC-SIS (Balasubramanian et al., 2013), KCCA-SIS is scale-free removing the marginal variation of features and response variables. Similar to DC-SIS and sup-HSIC-SIS, KCCA-SIS can also be used directly to screen grouped predictors and handle multivariate response variables. We show that KCCA-SIS has the sure screening property, and has better performance through simulation studies and its application to a brain gene expression dataset.

**Keywords:** Sure independence screening, Kernel canonical correlation analysis, Model-free, Reproducing Kernel Hilbert Space, Human brain gene expression

## 1. Introduction

Ultrahigh dimensional data sets have become common in many disciplines. For example, the reducing cost in microarrays and sequencing allows researchers to collect information on gene expression and sequence data at the whole genome level. A typical study may generate expression information from tens of thousands of genes (denoted as  $p$ ) across dozens to hundreds of subjects (denoted as  $n$ ). Feature screening is important in genetics/genomics

studies to identify disease genes, construct gene networks, and develop biomarkers. Various regularization methods have been proposed and their statistical properties studied for these high dimensional problems, such as: Lasso (Tibshirani, 1996), Dantzig selector (Candes and Tao, 2007), SCAD (Fan and Li, 2001), and MCP (Zhang, 2010). All of these methods allow the number of selected predictors to be larger than sample size.

However, the above mentioned methods may not perform well for ultrahigh dimensional data due to the simultaneous challenges in computational efficiency, statistical consistency and algorithmic robustness (Zhao and Yu (2006), Fan et al. (2009), Fan and Lv (2010)). In order to tackle these difficulties, (Fan and Lv, 2008) proposed the Sure Independence Screening (SIS) and showed that the Pearson correlation ranking procedure possesses a sure screening property for linear regressions with Gaussian predictors and responses. Since the publication of SIS, several extensions were made to consider generalized linear models (Fan et al., 2009) and nonparametric independence screening in sparse ultrahigh dimensional additive models (Fan et al., 2011). Ji et al. (2012) further proposed a two-stage method called UPS: screening by univariate thresholding and cleaning by penalized least squares for selecting variables. Li et al. (2012) proposed DC-SIS, a sure independence screening model-free method based on distance correlation as a measure of relationship between response and covariate. Song et al. (2012) proposed a method based on Hilbert–Schmidt Independence Criterion (HSIC, for short). To generalize the idea of DC-SIS, Balasubramanian et al. (2013) proposed a general framework, called sup-HSIC-SIS, for model-free and multi-output screening. Motivated from the equivalence between distance covariance and HSIC (Sejdinovic et al., 2013), they used Reproducing Kernel Hilbert Space (RKHS) based independence measures (Gretton et al., 2005).

In this paper, we propose a new method called Kernel Canonical Correlation Analysis (KCCA)-SIS, which removes the marginal effect of variables compared to sup-HSIC-SIS and DC-SIS. HSIC calculates the maximum covariance between the transformations of two random variables restricted in certain function classes, while KCCA calculates the maximum correlation between the transformed ones by removing the marginal variations of random variables. KCCA (Akaho (2006), Melzer et al. (2001), Bach and Jordan (2003)) was first proposed as a nonlinear extension of canonical correlation aiming to extract the shared information between two random variables, i.e., to provide nonlinear mappings  $f \in \mathcal{H}_X$  and  $g \in \mathcal{H}_Y$  so that  $\text{cor}[f(X), g(Y)]$  is maximized. It was shown in Fukumizu et al. (2007a) that the maximum of the objective function in KCCA is identical to the operator norm of the correlation operator between  $\mathcal{H}_X$  and  $\mathcal{H}_Y$ . This fact motivates us to use the operator norm of the correlation operator as a measure for the relationship between random variables. We show that KCCA-SIS enjoys the sure screening property under mild conditions. In both simulations and a real data application for extracting interneuron related genes in the human brain, we show that the proposed method performs better than the existing approaches.

The rest of this paper is organized as follows. In Section 2, we develop the KCCA-SIS for feature screening and establish its sure screening property. In Section 3, we compare the proposed method with other approaches on simulated and real data. We conclude this paper with a brief discussion in Section 4. All technical proofs are given in the Appendix.

## 2. Independence screening using Kernel CCA

### 2.1 Some Preliminaries

Let  $(\mathcal{X}, \mathcal{B}_{\mathcal{X}})$  and  $(\mathcal{Y}, \mathcal{B}_{\mathcal{Y}})$  denote Borel measurable spaces. For example, they can be  $\mathbb{R}^d$  or any topological Borel measurable spaces. Given positive definite kernels  $k_x$  and  $k_y$ , let  $(\mathcal{H}_X, k_x)$  and  $(\mathcal{H}_Y, k_y)$  be RKHSs (Aronszajn, 1950) of functions on  $\mathcal{X}$  and  $\mathcal{Y}$ , respectively. We denote the marginal distributions of  $X$  and  $Y$  as  $\mathbb{P}_X$  and  $\mathbb{P}_Y$ , and their joint distribution as  $\mathbb{P}_{XY}$ . We denote the expectation operator associated with  $\mathbb{P}_X$ ,  $\mathbb{P}_Y$ , and  $\mathbb{P}_{XY}$  as  $\mathbb{E}_X$ ,  $\mathbb{E}_Y$ , and  $\mathbb{E}_{XY}$ , respectively. For a random variable  $X : \Omega \rightarrow \mathcal{X}$ , the *mean element*  $m_X \in \mathcal{H}_X$  is induced by the relation, for all  $f \in \mathcal{H}_X$

$$\langle f, m_X \rangle_{\mathcal{H}_X} = \mathbb{E}_X[\langle k_x(\cdot, X), f \rangle] = \mathbb{E}_X f(X),$$

where  $\langle \cdot, \cdot \rangle_{\mathcal{H}_X}$  denotes the inner product under  $\mathcal{H}_X$ . By the Riesz representation theorem (Reed and Simon, 1980), there exists an operator  $\Sigma_{YX} : \mathcal{H}_X \rightarrow \mathcal{H}_Y$  so that

$$\langle g, \Sigma_{YX} f \rangle_{\mathcal{H}_Y} = \mathbb{E}_{XY}[\langle f, k_x(\cdot, X) - m_X \rangle_{\mathcal{H}_X} \langle k_y(\cdot, Y) - m_Y, g \rangle_{\mathcal{H}_Y}] = \text{Cov}(f(X), g(Y))$$

holds for all  $f \in \mathcal{H}_X$  and  $g \in \mathcal{H}_Y$ . We call this operator *cross-covariance operator* (Fukumizu et al., 2009). If  $Y$  is equal to  $X$ , the positive self-adjoint operator  $\Sigma_{XX}$  is called the *covariance operator*. Baker (1973, Theorem 1) showed that  $\Sigma_{YX}$  can be expressed as

$$\Sigma_{YX} = \Sigma_{YY}^{1/2} \mathcal{R}_{YX} \Sigma_{XX}^{1/2}, \quad (1)$$

where  $\mathcal{R}_{YX} : \mathcal{H}_X \rightarrow \mathcal{H}_Y$  is a unique bounded operator such that  $\|\mathcal{R}_{YX}\| \leq 1$ . We call  $\mathcal{R}_{YX}$  the *correlation operator* from  $\mathcal{H}_X$  to  $\mathcal{H}_Y$ , capturing all the nonlinear information between  $X$  and  $Y$ . On the other hand, assuming  $k : (\mathcal{X} \times \mathcal{Y})^2 \rightarrow \mathbb{R}$  to be separable, i.e.,  $k((x, y), (x', y')) = k_x(x, x')k_y(y, y')$ , where  $k_x : \mathcal{X}^2 \rightarrow \mathbb{R}$  and  $k_y : \mathcal{Y}^2 \rightarrow \mathbb{R}$  are reproducing kernels of  $\mathcal{H}_X$  and  $\mathcal{H}_Y$  respectively (in which case  $\mathcal{H}$  is homomorphism to the tensor product of  $\mathcal{H}_X$  and  $\mathcal{H}_Y$ . i.e.,  $\mathcal{H} \cong \mathcal{H}_X \otimes \mathcal{H}_Y$ ), the Hilbert–Schmidt independence criterion (HSIC) is defined as  $\text{HSIC}(\mathbb{P}_{XY}, \mathcal{H}_X, \mathcal{H}_Y) := \|\Sigma_{XY}\|_{\text{HS}}^2$ , where  $\|\cdot\|_{\text{HS}}$  denotes the Hilbert–Schmidt norm of the operator. HSIC was first introduced by Gretton et al. (2005) and the authors showed that it can be represented as:

$$\begin{aligned} \text{HSIC}(\mathbb{P}_{XY}, \mathcal{H}_X, \mathcal{H}_Y) &= \mathbb{E}_{XX'YY'}[k_x(X, X')k_y(Y, Y')] + \mathbb{E}_{XX'}[k_x(X, X')]\mathbb{E}_{YY'}[k_y(Y, Y')] \\ &\quad - 2\mathbb{E}_{XY}[\mathbb{E}_{X'}[k_x(X, X')]\mathbb{E}_{Y'}[k_y(Y, Y')]], \end{aligned}$$

where  $(X', Y')$  are an independent copy of  $(X, Y)$  and  $\mathbb{E}_{XX'YY'}$  denotes the expectation over the independent pairs. Under the condition that  $k_x$  and  $k_y$  are characteristic (Fukumizu et al., 2007b),  $\text{HSIC}(\mathbb{P}_{XY}, \mathcal{H}_X, \mathcal{H}_Y)$  is zero iff  $X$  and  $Y$  are independent. From this, we know that  $\|\Sigma_{YX}\| = 0$  iff  $X$  and  $Y$  are independent, where  $\|\cdot\|$  denotes the operator norm. Furthermore, it is easy to show that  $\|\mathcal{R}_{YX}\| = 0$  iff  $X$  and  $Y$  are independent (Fukumizu et al., 2007b).

With a slight abuse of notation, we write  $\mathcal{R}_{YX} = \Sigma_{YY}^{-1/2} \Sigma_{YX} \Sigma_{XX}^{-1/2}$ , where  $\Sigma_{YY}$  and  $\Sigma_{XX}$  may not be invertible. We define the regularized version of  $\mathcal{R}_{YX}$  as

$$\mathcal{R}_{YX}(\epsilon_n) \triangleq (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX} (\Sigma_{XX} + \epsilon_n I)^{-1/2},$$

where  $\epsilon_n > 0$  is the ridge parameter Fukumizu et al. (2007a, Lemma 7) showed that if  $\mathcal{R}_{YX}$  is compact,

$$\|\mathcal{R}_{YX}(\epsilon_n) - \mathcal{R}_{YX}\| \rightarrow 0, \text{ as } \epsilon_n \rightarrow 0.$$

Next we derive a sample level estimator of  $\mathcal{R}_{YX}(\epsilon_n)$ . Suppose  $\{(X^{(i)}, Y^{(i)})\}_{i=1}^n$  is a set of  $n$  independent copies from  $(X, Y)$ . Then the *empirical cross-covariance operator*  $\hat{\Sigma}_{YX}^{(n)}$  is defined as the cross-covariance operator under the empirical distribution  $\frac{1}{n} \sum_{i=1}^n \delta_{X^{(i)}} \delta_{Y^{(i)}}$ , where  $\delta_{X^{(i)}}$  and  $\delta_{Y^{(i)}}$  are Dirac measures with point mass on  $X^{(i)}$  and  $Y^{(i)}$ . That is, for any  $f \in \mathcal{H}_X$  and  $g \in \mathcal{H}_Y$ ,  $\hat{\Sigma}_{YX}^{(n)}$  satisfies

$$\langle g, \hat{\Sigma}_{YX}^{(n)} f \rangle_{\mathcal{H}_Y} = \text{Cov}_n[f(X), g(Y)],$$

where  $\text{Cov}_n(X, Y)$  is the empirical covariance between two random variables with respect to the empirical measure. We can similarly define  $\hat{\Sigma}_{YY}^{(n)}$  and  $\hat{\Sigma}_{XX}^{(n)}$ . We then have the regularized estimator of  $\mathcal{R}_{YX}$ :

$$\hat{\mathcal{R}}_{YX}^{(n)}(\epsilon_n) \triangleq (\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-1/2} \hat{\Sigma}_{YX}^{(n)} (\hat{\Sigma}_{XX}^{(n)} + \epsilon_n I)^{-1/2}.$$

Empirically, we use  $\|\hat{\mathcal{R}}_{YX}^{(n)}(\epsilon_n)\|$  as the measure of dependency between predictor  $X$  and response  $Y$ .  $\hat{\mathcal{R}}_{YX}^{(n)}(\epsilon_n)$  was first introduced in Fukumizu et al. (2007a) and is called the normalized cross-covariance operator (NOCCO)

## 2.2 An Independence Ranking and Screening Procedure

In this section we propose an independence screening procedure based on KCCA. We assume a response  $Y \in \mathbb{R}^d$  and predictors  $X \in \mathbb{R}^p$ , with  $p$  growing with  $n$  and  $d$  fixed. It is often assumed that only a small number of predictors are relevant to  $Y$ .

Denote by  $\mathbb{P}(Y|X)$  the conditional distribution of  $Y$  given  $X$ . Following (Li et al., 2012), we define the set of relevant variables called *active set*  $\mathcal{M}$  and irrelevant variables called *inactive set*  $\mathcal{I}$  as:

$$\begin{aligned} \mathcal{M} &= \{r : \mathbb{P}(Y|X) \text{ depends on } X_r\}, \text{ and} \\ \mathcal{I} &= \{r : \mathbb{P}(Y|X) \text{ does not depend on } X_r\}. \end{aligned}$$

We write  $X_{\mathcal{M}} = \{X_r : r \in \mathcal{M}\}$  and  $X_{\mathcal{I}} = \{X_r : r \in \mathcal{I}\}$ , and call  $X_{\mathcal{M}}$  as an *active predictor vector* and its complement  $X_{\mathcal{I}}$  as an *inactive predictor vector*. By the definition we know that  $Y$  and  $X_{\mathcal{I}}$  are independent conditional on  $X_{\mathcal{M}}$ . In this case, feature selection involves estimating the set  $\mathcal{M}$  from the given  $n$  samples.

A direct way is to rank the predictors according to their degree of dependence with the response. We consider the norm of correlation operator as a measure of such dependence. To be specific, we write

$$\rho_r(\epsilon_n) = \|(\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\|,$$

to be the measure of dependence between  $X_r$  and  $Y$ , because  $\rho_r(\epsilon_n) = 0$  for any  $\epsilon_n > 0$  iff  $X_r$  and  $Y$  are independent. Similar to distance correlation, our measure here is model-free and allows for multivariate response and group predictors. Similar to sup-HSIC-SIS, our method can be used in the case of more general topological space for response  $Y$ .

## 2.3 The learning algorithm

### 2.3.1 CHOICE OF KERNEL

As mentioned before, we choose Gaussian kernel for its universal property. The form of Gaussian kernel is defined as:

$$k(x, y) = \exp(-\gamma \|x - y\|_2^2),$$

where  $\|\cdot\|_2$  stands for Euclidean norm.

In sample version, we have the corresponding estimator  $\hat{\rho}_r(\epsilon_n) = \|\hat{\mathcal{R}}_{YX_r}^{(n)}(\epsilon_n)\|$ . In order to select the relevant variables, we first compute  $\hat{\rho}_r(\epsilon_n)$  for  $r = 1, \dots, p$  and define

$$\hat{\mathcal{M}} = \{r : \hat{\rho}_r(\epsilon_n) \geq C_3 \epsilon_n^{-3/2} n^{-\kappa}, \text{ for } 1 \leq r \leq p\}$$

as the estimated set of active predictors, where  $0 \leq \kappa < 1/2$ ,  $C_3$  is predefined constant in condition (C2) and  $\epsilon_n^{-3/2}$  is due to some technical issues explained later.

### 2.3.2 SAMPLE LEVEL ESTIMATOR

Following Lee et al. (2016), we will derive the empirical representation of  $\|\hat{\mathcal{R}}_{YX_r}^{(n)}(\epsilon_n)\|$ , where  $Y \in \mathbb{R}^d$  and  $X_r \in \mathbb{R}$ . Suppose we observe  $n$  i.i.d samples  $(X_r^{(1)}, Y^{(1)}), \dots, (X_r^{(n)}, Y^{(n)})$ , let  $K_{X_r}, K_Y$  be two positive semidefinite kernel matrices with  $(K_{X_r})_{ij} = k(X_r^{(i)}, X_r^{(j)})$  and  $(K_Y)_{ij} = k(Y^{(i)}, Y^{(j)})$ . Let  $Q = I_n - \frac{1}{n} \mathbf{1}\mathbf{1}^T$ ,  $G_{X_r} = QK_{X_r}Q$ , and  $G_Y = QK_YQ$ . Let the singular value decompositions of  $G_{X_r}$  and  $G_Y$  be  $U_{X_r}D_{X_r}U_{X_r}^T$  and  $U_YD_YU_Y^T$ , respectively. Here  $U_{X_r}, D_{X_r}, U_Y, D_Y \in \mathbb{R}^{n \times n}$ . We use  $A^\dagger$  to denote the Moore-Penrose inverse of a matrix  $A$ , and  $A^{\dagger\alpha}$  to denote  $(A^\dagger)^\alpha$ . We choose the orthonormal basis

$$(\phi_1, \dots, \phi_{r_x}) = (k_{x_r}(\cdot, X_r^{(1)}), \dots, k_{x_r}(\cdot, X_r^{(n)}))QU_{X_r}D_{X_r}^{\dagger 1/2}$$

and

$$(\psi_1, \dots, \psi_{r_y}) = (k_y(\cdot, Y^{(1)}), \dots, k_y(\cdot, Y^{(n)}))QU_YD_Y^{\dagger 1/2}.$$

Then we can represent  $f = (\phi_1, \dots, \phi_{r_x})[f]$  for  $[f] \in \mathbb{R}^n$  and

$$(f(X_r^{(1)}), \dots, f(X_r^{(n)}))^T = K_{X_r}QU_{X_r}D_{X_r}^{\dagger 1/2}[f]. \quad (2)$$

The notation  $[\cdot]$  is the coordinate with respect to the new basis system; Lee et al. (2013) and Lee et al. (2016) also adopted a similar coordinate system. We denote  $\mathcal{H}_{X_r}^{(n)} \subseteq \mathcal{H}_{X_r}$  to be the RKHS generated by  $(k_{x_r}(\cdot, X_r^{(1)}), \dots, k_{x_r}(\cdot, X_r^{(n)}))$  and similarly for  $\mathcal{H}_Y^{(n)} \subseteq \mathcal{H}_Y$ . Then for any two functions  $f_1, f_2 \in \mathcal{H}_{X_r}^{(n)}$

$$\langle f_1, f_2 \rangle_{\mathcal{H}_{X_r}} = [f_1]^T D_{X_r}^{\dagger 1/2} U_{X_r}^T Q K_{X_r} Q U_{X_r} D_{X_r}^{\dagger 1/2} [f_2] = [f_1]^T [f_2].$$

For  $f \in \mathcal{H}_{X_r}^{(n)}$  and  $g \in \mathcal{H}_Y^{(n)}$ ,

$$\begin{aligned} [g]^T [\hat{\Sigma}_{YX_r}^{(n)}][f] &= \langle g, \hat{\Sigma}_{YX_r}^{(n)} f \rangle_{\mathcal{H}_Y} = (g(Y_1), \dots, g(Y_n))^T Q (f(X_{r1}), \dots, f(X_{rn})) \\ &= [g]^T D_Y^{\dagger 1/2} U_Y^T Q K_Y Q Q K_{X_r} Q U_{X_r} D_{X_r}^{\dagger 1/2} [f] \\ &= [g]^T D_Y^{\dagger 1/2} U_Y^T U_{X_r} D_{X_r}^{\dagger 1/2} [f], \end{aligned}$$

where the second equality follows from equation (2). So we have  $[\hat{\Sigma}_{YX_r}^{(n)}] = D_Y^{1/2} U_Y^T U_{X_r} D_{X_r}^{1/2}$ ,  $[\hat{\Sigma}_{YY}^{(n)}] = D_Y$ ,  $[\hat{\Sigma}_{X_r X_r}^{(n)}] = D_{X_r}$ . Then we can easily show that

$$[\hat{\mathcal{R}}_{YX_r}^{(n)}(\epsilon_n)] = (D_Y + \epsilon_n I)^{-1/2} D_Y^{1/2} U_Y^T U_{X_r} D_{X_r}^{1/2} (D_{X_r} + \epsilon_n I)^{-1/2}. \quad (3)$$

Since we just conduct the orthogonal transformation of the original matrix, the operator norm of sample correlation operator is just the largest singular value of  $[\hat{\mathcal{R}}_{YX_r}^{(n)}]$ .

### 2.3.3 TUNING PARAMETER SELECTION

For Gaussian kernel, we need to choose the bandwidth parameter  $\gamma$ . For  $i = 1, \dots, p$ , we compute  $\gamma_i$  via

$$\frac{1}{\sqrt{\gamma_i}} = \frac{2\sqrt{2}}{n(n-1)} \sum_{i < j} \|X^{(i)} - X^{(j)}\|_2. \quad (4)$$

Similarly we can compute  $\gamma_Y$  for  $Y$ .

For the choice of  $\epsilon_n$ , we use a generalized cross-validation (GCV) criterion similar to Li et al. (2014). To be specific, let  $L_Y = (\mathbf{1}, K_Y)^T$ ,  $L_r = (\mathbf{1}, K_{X_r})^T$ , where  $K_Y$  and  $K_{X_r}$  are the corresponding kernel matrices. Then we define

$$\text{GCV}(\epsilon_n) = \sum_{r=1}^p \frac{\|L_Y - L_Y L_r^T (L_r L_r^T + \epsilon_n I_{n+1})^{-1} L_r\|_F^2}{\{1 - \text{tr}(L_r^T (L_r L_r^T + \epsilon_n I_{n+1})^{-1} L_r)/n\}^2}, \quad (5)$$

where  $\|\cdot\|_F$  is the Frobenius norm of a matrix. We choose  $\epsilon_n$  by minimizing  $\text{GCV}(\epsilon_n)$ .

### 2.3.4 FEATURE SCREENING PROCEDURE

The algorithm is as follows:

- (a) Calculate the bandwidth parameters  $\gamma_1, \dots, \gamma_p$ , and  $\gamma_Y$  using (4);
- (b) Calculate the ridge parameter  $\epsilon_n$  determined by (5) by grid search in the set  $\{10^{-5}, 10^{-4}, \dots, 10^3\}$ ;
- (c) Compute the gram matrices  $G_Y, G_{X_1}, \dots, G_{X_p}$  based on the Gaussian kernel function, and find their singular value decompositions;
- (d) Compute the norm of  $[\hat{\mathcal{R}}_{YX_i}^{(n)}(\epsilon_n)]$  based on (3);
- (e) Rank  $\|[\hat{\mathcal{R}}_{YX_i}^{(n)}(\epsilon_n)]\|$  for  $i = 1, \dots, p$ . Suppose  $\|[\hat{\mathcal{R}}_{YX_{r_1}}^{(n)}(\epsilon_n)]\| \geq \dots \geq \|[\hat{\mathcal{R}}_{YX_{r_p}}^{(n)}(\epsilon_n)]\|$ ; we then estimate  $\mathcal{M}$  by  $\hat{\mathcal{M}} = \{r_1, \dots, r_m\}$ .

In practice, the choice of  $m$  may depend on the researchers' prior knowledge and also the sample size. In our simulation analysis, we use different numbers of  $m$  based on the true number of active predictors. In our real data analysis, we choose the upper 1% as active predictors. Empirically, we recommend using  $1.5\epsilon_n^{-3/2} n^{1/4}$ , where  $\epsilon_n$  is the best tuning parameter chosen by (5).

## 2.4 Theoretical Guarantees

In this section, we study the theoretical properties of the proposed independence screening method. Our analysis does not require any moment conditions on the variables  $X$  and  $Y$  such as spherical symmetric distribution in Fan and Lv (2008), or sub-gaussian in Li et al. (2012). Instead, we require the following two conditions:

(C1) The uniform boundedness of kernel functions:

$$\sup_{1 \leq r \leq p} k_{x_r}(x, x) \leq B < \infty, \quad k_y(y, y) \leq B < \infty \quad (6)$$

(C2) The minimum signal strength condition:

$$\min_{r \in \mathcal{M}} \rho_r(\epsilon_n) \geq 2C_3 \epsilon_n^{-3/2} n^{-\kappa}, \quad (7)$$

for some constants  $C_3 > 0$  specified in Theorem 2.3 and  $0 \leq \kappa < 1/2$ .

Note that condition (C1) holds for many commonly used kernels, such as the radial basis function. Condition (C2) requires that KCCA measure corresponding to the active predictors cannot be too weak, which is an analog of condition 3 of Fan and Lv (2008). First, we have a concentration bound for cross-covariance operator as in Theorem 2.1:

**Theorem 2.1.** *Suppose (C1) holds, then we have for  $r = 1, \dots, p$ ,*

$$\mathbb{P}\{\|\hat{\Sigma}_{YX_r} - \Sigma_{YX_r}\|_{\text{HS}} - \mathbb{E}\|\hat{\Sigma}_{YX_r} - \Sigma_{YX_r}\|_{\text{HS}} \geq t\} \leq \exp(-\frac{C_2 n t^2}{B^2}).$$

Based on the concentration bound in Theorem 2.1, we can establish the following concentration bound for the correlation operator:

**Theorem 2.2.** *Suppose (C1) holds,  $\epsilon_n = o(1)$  and  $n^{-1} \epsilon_n^{-3} = o(1)$ . Then there exist constants  $C_1, C_2 > 0$ , such that*

$$\begin{aligned} \mathbb{P}\{&\|\hat{\mathcal{R}}_{YX_r}^{(n)}(\epsilon_n) - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\| \\ &- C_1 K^{3/2} \epsilon_n^{-3/2} n^{-1/2} \geq t\} \leq 3 \exp(-\frac{C_2 \epsilon_n^3 n t^2}{B^2}), \end{aligned}$$

for  $r = 1, \dots, p$ .

Based on the concentration bounds and conditions (C1) and (C2), we can achieve the following sure independence screening property.

**Theorem 2.3.** *Suppose (C1) holds, there exist constants  $C_3, C_4 > 0$ ,  $0 \leq \kappa < 1/2$  such that*

$$\mathbb{P}\{\max_{1 \leq r \leq p} |\hat{\rho}_r(\epsilon_n) - \rho_r(\epsilon_n)| \geq C_3 B^{3/2} \epsilon_n^{-3/2} n^{-\kappa}\} \leq 3p \exp(-C_4 B n^{1-2\kappa}).$$

Furthermore if condition (C2) holds, then we have the following sure screening property:

$$\mathbb{P}\{\mathcal{M} \subseteq \hat{\mathcal{M}}\} \geq 1 - 3s \exp(-C_4 B n^{1-2\kappa}),$$

where  $s$  is the cardinality of  $\mathcal{M}$ .



Based on the above result, we can handle the NP dimensionality  $\log p = o(n^{1-2\kappa})$ .

The sure screening property without controlling for false selection rates is not satisfactory. Ideally if there is a gap between active variables and inactive variables regarding their  $\rho(\epsilon_n)$ , i.e.  $\max_{j \notin \mathcal{M}} \rho_r(\epsilon_n) = o(B^{3/2} \epsilon_n^{3/2} n^{-\kappa})$ , the false-positive rate will vanish.

Next, we show that the size of  $\hat{\mathcal{M}}$  can be controlled when there is no severe dependency between the predictors. Suppose  $\mathcal{H}_X$  is the direct sum  $\oplus_{r=1}^p \mathcal{H}_{X_r}$ ; in other words,  $\mathcal{H}_X$  is induced by the additive kernel  $k_x(s, t) = \sum_{i=1}^p k_{x_r}(s_i, t_i)$ , for any  $s = (s_1, \dots, s_p)$  and  $t = (t_1, \dots, t_p)$ . It can be shown that the covariance operator  $\Sigma_{XX} : \mathcal{H}_X \rightarrow \mathcal{H}_X$  has a matrix form satisfying that, for any  $f = (f_1, \dots, f_p) \in \mathcal{H}_X$ ,

$$\Sigma_{XX} f = \sum_{r=1}^p \sum_{s=1}^p \Sigma_{X_r X_s} f_s.$$

Then the following result provides an upper bound for  $|\hat{\mathcal{M}}|$ .

**Theorem 2.4.** *For  $\epsilon_n \leq 1$ , we have*

$$\mathbb{P}\{|\hat{\mathcal{M}}| \leq O(n^{2\kappa} \lambda_{\max}(\Sigma_{XX}))\} \geq 1 - 3p \exp(-C_4 B n^{1-2\kappa}),$$

where  $\lambda_{\max}(\cdot)$  represents the largest singular value of the corresponding operator, and  $C_4 > 0$  is the constant in Theorem 2.3.

### 3. Numerical Results

In this section, we report results on different simulated and real biological data to illustrate the advantage of the propose method (KCCA-SIS). For the experiments on synthetic data, we consider the data settings from Li et al. (2012) and Balasubramanian et al. (2013) in order to make a head to head comparison to their approaches. For evaluation on real world data, we consider a high dimensional human brain gene expression data set, select genes related to marker genes for interneuron cells, and measure the performance of the selection using gene set enrichment analysis.

In simulations 1 and 2, we generate random vector  $X = (X_1, X_2, \dots, X_p)$  from a multivariate Gaussian distribution with zero mean and covariance matrix  $\Sigma = (\sigma_{ij})_{p \times p}$ , where  $\sigma_{ij} = 0.8^{|i-j|}$ . The error term  $\varepsilon$  is generated from  $N(0, 1)$ . We fix the sample size  $n$  to be 200 and number of features  $p$  to be 2000. We repeat each experiment 500 times, and evaluate the performance through the following two criteria (the same as those used in Li et al. (2012)).

- 1  $\mathcal{S}$ : the minimum model size to include all active predictors. We report the 25%, 50%, and 75% quantiles of  $\mathcal{S}$  using replications.
- 2  $\mathcal{P}$ : the proportion that all active predictors are selected for a given model size  $d$  in the 500 replications.

The metric  $\mathcal{S}$  is used as a measure of model complexity needed for sure screening with regard to the underlying screening procedure. The lower the value of  $\mathcal{S}$ , the better the screening procedure. The sure screening property ensures that  $\mathcal{P}$  is close to one when the estimated model size  $d$  is sufficiently large. We choose  $d$  to be  $d_1 = \lceil n / \log n \rceil$ ,  $d_2 = 2d_1$  and  $d_3 = 3d_1$  throughout our simulations, where  $\lceil c \rceil$  denotes the integer part of  $c$ .



### 3.1 Simulation 1

This example is designed to compare the finite sample performance of the KCCA-SIS with SIS (Fan and Lv, 2008), DC-SIS (Li et al., 2012) and HSIC-SIS (Balasubramanian et al., 2013). We generate the response  $Y$  according to four models (The first three models are used in Li et al. (2012)):

1.  $Y = c_1\beta_1X_1X_2 + c_3\beta_2\mathbb{1}(X_{12} < 0) + c_4\beta_3X_{22} + \varepsilon;$
2.  $Y = c_1\beta_1X_1X_2 + c_3\beta_2\mathbb{1}(X_{12} < 0)X_{22} + \varepsilon;$
3.  $Y = c_1\beta_1X_1 + c_2\beta_2X_2 + c_3\beta_3\mathbb{1}(X_{12} < 0) + \exp(c_4|X_{22}|)\varepsilon;$
4.  $Y = X_1/X_2 + X_{12}^2/(1 + \cos(X_{22})) + \varepsilon,$

where  $\beta_j = (-1)^U(a + |Z|)$ ,  $a = 4 \log n / \sqrt{n}$ ,  $U \sim \text{Bernoulli}(0.4)$  and  $Z \sim N(0, 1)$ . We set  $(c_1, c_2, c_3, c_4) = (2, 0.5, 3, 2)$  in this example. For each independence screening procedure, we compute the associated marginal effect of  $X_r$  on  $Y$ . In this case we treat  $X = (X_1, \dots, X_p)$  as the predictor variables. We use the GCV criterion to select  $\epsilon_n$ .

Tables 1 and 2 report the simulation results for  $\mathcal{S}$  and  $\mathcal{P}$ . We can observe that screening fails in all four models by SIS. The proposed method outperforms DC-SIS in all cases and HSIC-SIS in most cases. We notice that our proposed KCCA-SIS is better than DC-SIS, comparable with sup-HSIC-SIS in model 3, where there is heteroscedasticity. The better performance is likely due to the removal of the marginal variations of responses and predictors. We have similar results as HSIC-SIS for larger  $\epsilon_n$ . The advantage of the proposed approach is clearly demonstrated in model 4, where the marginal variations are different among predictors. In that case KCCA-SIS performs much better than the other methods.

$\mathcal{S}$	SIS			DC-SIS			HSIC-SIS			KCCA-SIS		
	25%	50%	75%	25%	50%	75%	25%	50%	75%	25%	50%	75%
1	208.3	818.0	1534.0	8.0	13.0	20.0	7.0	10.0	16.0	5.0	7.0	11.0
2	801.8	1302.0	1663.5	11.0	16.0	41.5	6.0	8.0	13.0	5.0	6.0	9.0
3	581.0	1135.0	1598.0	7.0	13.0	60.3	5.0	8.0	17.0	6.0	8.0	27.0
4	1534.0	1807.0	1924.3	385.8	770.5	1174.0	52.0	358.0	867.0	33.0	139.0	463.3

Table 1: Minimum model size ( $\mathcal{S}$ ) comparisons among different methods in simulation 1

$\mathcal{P}$	SIS			DC-SIS			HSIC-SIS			KCCA-SIS		
	$d_1$	$d_2$	$d_3$	$d_1$	$d_2$	$d_3$	$d_1$	$d_2$	$d_3$	$d_1$	$d_2$	$d_3$
1	0.08	0.14	0.17	0.90	0.96	0.97	0.92	0.95	0.97	0.94	0.96	0.97
2	0.00	0.01	0.02	0.73	0.86	0.91	0.92	0.95	0.96	0.95	0.97	0.98
3	0.01	0.03	0.05	0.70	0.77	0.80	0.84	0.88	0.90	0.78	0.85	0.87
4	0.00	0.00	0.00	0.00	0.01	0.04	0.06	0.12	0.20	0.21	0.30	0.37

Table 2: The proportions ( $\mathcal{P}$ ) comparisons among different methods in simulation 1

### 3.2 Simulation 2

In this experiment, we consider multivariate outputs, while  $X$  is generated as before. We generate  $Y|X \sim N(\mathbf{0}, \Sigma)$  from a bivariate normal distribution, where  $\sigma_{11} = \sigma_{22} = 1$  and  $\sigma_{12} = \sigma_{21} = \sigma(X)$ . We consider two correlation functions for  $\sigma(X)$  given by

1.  $\sigma(X) = \sin(\beta_1^T X)$  where  $\beta_1 = (0.8, 0.6, 0, \dots, 0)$ ;
2.  $\sigma(X) = \{\exp(\beta_2^T X) - 1\} / \{\exp(\beta_2^T X) + 1\}$  where  $\beta_2 = (2 - U_1, 2 - U_2, 2 - U_3, 2 - U_4, 0, \dots, 0)$  with  $U_i$  drawn i.i.d. from Uniform[0,1].

In model 1, we choose  $d_1 = 2$ . In model 2, we choose  $d_1 = 4$ . And we choose  $d_2 = 2d_1$  and  $d_3 = 3d_1$  as before. The simulation settings are identical to those in Li et al. (2012). Since the response is a vector, SIS cannot be applied in this scenario. The simulation results are shown in Table 3 and Table 4.

$\mathcal{S}$	DC-SIS			HSIC-SIS			KCCA-SIS		
Model	25%	50%	75%	25%	50%	75%	25%	50%	75%
1	3.0	7.0	16.0	2.0	2.0	3.0	2.0	2.0	2.0
2	4.0	5.0	7.0	4.0	4.0	4.0	4.0	4.0	4.0

Table 3: Minimum model size ( $\mathcal{S}$ ) comparisons among different methods in simulation 2

$\mathcal{P}$	DC-SIS			HSIC-SIS			KCCA-SIS		
Model	$d_1$	$d_2$	$d_3$	$d_1$	$d_2$	$d_3$	$d_1$	$d_2$	$d_3$
1	0.170	0.364	0.480	0.678	0.868	0.926	0.984	0.996	1.000
2	0.488	0.856	0.930	0.768	0.960	0.984	0.978	1.000	1.000

Table 4: The proportions ( $\mathcal{P}$ ) comparisons among different methods in simulation 2

### 3.3 Real data

In this subsection, we analyze a brain spatial temporal gene expression data set from Kang et al. (2011). We consider gene expression data from 10 neocortex areas (MFC, OFC, DFC, VFC, M1C, S1C, IPC, A1C, STC, ITC) at 13 developmental stages (early fetal to late adulthood). For each gene, there are  $10 \times 13 = 130$  observations corresponding to a spatial temporal characterization of this gene. There are a total of 17568 genes. Zeisel et al. (2015) reported newly identified marker genes for interneuron cell types using single cell RNA sequencing on mouse brain. We use those marker genes, including SP8, POU3F4, TOX3, NPAS1, SOX6, NKX2-1, LHX6, PAX6, DLX5, ARX, DLX2, DLX1, ELAVL2, and SP9, as the response variable. Interneurons have been found to function in reflexes, neuronal oscillations, and neurogenesis in the adult mamalian brain (Kandel et al., 2000). And Zeng et al. (2012) found that the interneuron marker genes are conserved between mouse and human, thus we apply the identified marker genes directly as response variables in human brain gene expression data set. Since this is a multivariate response, we can use

DC-SIS, HSIC-SIS, and KCCA-SIS to select predictions. We select the top 1 percent of genes (i.e.,  $|\hat{\mathcal{M}}| = 176$ ) related to the above marker genes (including themselves), and then conduct gene enrichment analysis (<http://geneontology.org/page/go-enrichment-analysis>). We choose the union of five most significant biological processes. The results of fold-change and p-value related to biological processes for each method are shown in Table 5. We can see that KCCA-SIS captures more biologically meaningful genes as reflected in lower p-values. For neurogenesis, KCCA-SIS identifies 43 enriched genes, while DC-SIS identifies 36 and HSIC-SIS identifies 38 genes, respectively. KCCA-SIS is more powerful in selecting genes with similar biological functions. Besides, KCCA-SIS leads to 45 significant enrichment biological process terms, while DC-SIS leads to 16 terms and HSIC-SIS leads to 21 terms. This suggests that the results provided by KCCA-SIS are more biologically meaningful.

Biological Process	DC-SIS	HSIC-SIS	KCCA-SIS
nervous system development	6.56E-05	3.37E-06	9.68E-11
central nervous system development	1.00E00	1.00E00	1.19E-10
neurogenesis	6.48E-04	1.20E-04	4.80E-08
single-multicellular organism process	4.12E-06	2.51E-05	5.12E-08
head development	1.00E00	1.00E00	1.02E-07
multicellular organismal process	5.14E-04	9.56E-04	5.07E-07
anatomical structure development	6.60E-04	1.51E-03	5.62E-06
system development	1.09E-03	1.93E-04	9.90E-06
regulation of biological process	3.75E-03	2.77E-04	7.01E-04

Table 5: Gene Ontology enrichment analysis

#### 4. Discussion

In this article we have proposed an ultrahigh dimensional feature selection method via Kernel Canonical Correlation Analysis. The proposed approach is scale-free, model-free and works with multivariate random variables. We established the sure screening property of the proposed method and illustrated its capability in handling ultrahigh dimensional data on various simulated and real biological data sets.

Future work includes a theoretical analysis of the choice of thresholding and combination of KCCA-SIS and other nonlinear regression methods for a better predictive model.

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## Appendix A.

### A.1 Some useful lemmas

**Lemma A.1** (Fukumizu et al. (2007a)). *Suppose  $A$  and  $B$  are positive self-adjoint operators on Hilbert space such that  $0 \leq A \leq \lambda I$  and  $0 \leq B \leq \lambda I$  hold for a positive constant  $\lambda$ . Then,*

$$\|A^{3/2} - B^{3/2}\| \leq 3\lambda^{1/2}\|A - B\|.$$

**Lemma A.2** (Fukumizu et al. (2007a)). *The cross-covariance operator  $\Sigma_{YX}$  is a Hilbert-Schmidt operator, and its Hilbert-Schmidt norm is given by*

$$\begin{aligned} \|\Sigma_{YX}\|_{\text{HS}}^2 &= \mathbb{E}_{YX} \mathbb{E}_{\tilde{Y}\tilde{X}} [\langle k_x(\cdot, X) - m_X, k_y(\cdot, \tilde{X}) - m_X \rangle_{\mathcal{H}_X} \langle k_y(\cdot, Y) - m_Y, k_y(\cdot, \tilde{Y}) - m_Y \rangle_{\mathcal{H}_Y}] \\ &= \|\mathbb{E}_{YX} [(k_x(\cdot, X) - m_X)(k_y(\cdot, Y) - m_Y)]\|_{\mathcal{H}_X \otimes \mathcal{H}_Y}^2, \end{aligned}$$

where  $(\tilde{X}, \tilde{Y})$  and  $(X, Y)$  are independently and identically distributed with distribution  $P_{XY}$ .

Let's consider a fixed predictor  $X_r$  first. Let's denote  $F_r = k_{x_r}(\cdot, X_r) - \mathbb{E}_{X_r}[k_{x_r}(\cdot, X_r)]$ ,  $G = k_y(\cdot, Y) - \mathbb{E}_Y[k_y(\cdot, Y)]$ . For given i.i.d data  $\{(X^{(i)}, Y^{(i)})\}_{i=1}^n$ ,  $F_{ri} = k_{x_r}(\cdot, X_r^{(i)}) - \mathbb{E}_{X_r}[k_{x_r}(\cdot, X_r)]$ ,  $G_i = k_y(\cdot, Y^{(i)}) - \mathbb{E}_Y[k_y(\cdot, Y)]$ , and  $\mathcal{F}_r = \mathcal{H}_{X_r} \otimes \mathcal{H}_Y$  with kernel  $k((x, y), (x', y')) = k_{x_r}(x, x')k_y(y, y')$ . Then,  $F_r, F_{r1}, \dots, F_{rn}$  are i.i.d random elements in  $\mathcal{H}_{X_r}$ , and a similar fact holds for  $G, G_1, \dots, G_n$ . Notice that mean elements can be written as  $m_{X_r} = \mathbb{E}_{X_r}k_{x_r}(\cdot, X_r)$ ,  $m_Y = \mathbb{E}_Yk_y(\cdot, Y)$  (Fukumizu et al., 2007a).

**Lemma A.3.** *Under assumptions that  $\sup k_{x_r}(x, x) \leq B < \infty$ ,  $k_y(y, y) \leq B < \infty$ , we have for  $r = 1, \dots, p$  and  $i = 1, \dots, n$ ,*

$$\begin{aligned} \|F_{ri}\|_{\mathcal{H}_{X_r}} &\leq 2\sqrt{B}, \quad \|G_i\|_{\mathcal{H}_Y} \leq 2\sqrt{B}, \\ \|F_{ri} - F'_{ri}\|_{\mathcal{H}_{X_r}} &\leq 2\sqrt{B}, \quad \|G_i - G'_i\|_{\mathcal{H}_Y} \leq 2\sqrt{B}, \\ \|m_{X_r}\|_{\mathcal{H}_{X_r}} &\leq \sqrt{B}, \quad \|m_Y\|_{\mathcal{H}_Y} \leq \sqrt{B}. \end{aligned}$$

*Proof.*

$$\|F_{ri}\|_{\mathcal{H}_{X_r}} = \|k_{x_r}(\cdot, X_r) - m_{X_r}\|_{\mathcal{H}_{X_r}} \leq \|k_{x_r}(\cdot, X_r)\|_{\mathcal{H}_{X_r}} + \|m_{X_r}\|_{\mathcal{H}_{X_r}} \leq \sqrt{B} + \sqrt{B} = 2\sqrt{B},$$

where the first inequality comes from triangle inequality and the second from the definition of  $B$  and  $\|\cdot\|_{\mathcal{H}_{X_r}}$ . Using the similar techniques, we have

$$\|F_{ri} - F'_{ri}\|_{\mathcal{H}_X} = \|k_{x_r}(\cdot, X_r) - k_{x_r}(\cdot, X'_r)\|_{\mathcal{H}_{X_r}} \leq \|k_{x_r}(\cdot, X_r)\|_{\mathcal{H}_{X_r}} + \|k_{x_r}(\cdot, X'_r)\|_{\mathcal{H}_{X_r}} \leq 2\sqrt{B}.$$

By Cauchy-Schwartz inequality we have

$$\begin{aligned} \|m_{X_r}\|_{\mathcal{H}_{X_r}}^2 &= \langle \mathbb{E}_{X_r}k(\cdot, X_r), \mathbb{E}_{X'_r}k(\cdot, X'_r) \rangle \leq \mathbb{E}_{X_r}\mathbb{E}_{X'_r}k(X_r, X_r)^{1/2}k(X'_r, X'_r)^{1/2} \\ &\leq (\mathbb{E}_{X_r}k(X_r, X_r))^{1/2}(\mathbb{E}_{X'_r}k(X'_r, X'_r))^{1/2} \leq B. \end{aligned}$$

This completes the proof.  $\square$

**Lemma A.4.** *Under assumptions that  $\sup k_{x_r}(x, x) \leq B < \infty$ ,  $k_y(y, y) \leq B < \infty$ , we have for  $r = 1, \dots, p$ ,*

$$\mathbb{E} \|\hat{\Sigma}_{YX_r}^{(n)} - \Sigma_{YX_r}\|_{\text{HS}} \leq c_1 B n^{-1/2}, \mathbb{E} \|\hat{\Sigma}_{X_r X_r}^{(n)} - \Sigma_{X_r X_r}\|_{\text{HS}} \leq c_1 B n^{-1/2}, \mathbb{E} \|\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY}\|_{\text{HS}} \leq c_1 B n^{-1/2}$$

for some positive constant  $c_1$ . And

$$\begin{aligned} \|\Sigma_{YX_r}\|_{\text{HS}} &\leq 4B, \quad \|\Sigma_{X_r X_r}\|_{\text{HS}} \leq 4B, \quad \|\Sigma_{YY}\|_{\text{HS}} \leq 4B, \\ \|\hat{\Sigma}_{YX_r}\|_{\text{HS}} &\leq 8B, \quad \|\hat{\Sigma}_{X_r X_r}\|_{\text{HS}} \leq 8B, \quad \|\hat{\Sigma}_{YY}\|_{\text{HS}} \leq 8B. \end{aligned}$$

*Proof.* Following the same argument as in Fukumizu et al. (2007a), Lemma A.2 implies

$$\|\hat{\Sigma}_{YX_r}^{(n)}\|_{\text{HS}}^2 = \left\| \frac{1}{n} \sum_{i=1}^n \left( F_{ri} - \frac{1}{n} \sum_{j=1}^n F_{rj} \right) \left( G_i - \frac{1}{n} \sum_{j=1}^n G_j \right) \right\|_{\mathcal{F}_r}^2. \quad (8)$$

Using the argument in the proof of the same lemma,

$$\langle \Sigma_{YX_r}, \hat{\Sigma}_{YX_r}^{(n)} \rangle_{\text{HS}} = \left\langle \mathbb{E}[F_r G], \frac{1}{n} \sum_{i=1}^n \left( F_{ri} - \frac{1}{n} \sum_{j=1}^n F_{rj} \right) \left( G_i - \frac{1}{n} \sum_{j=1}^n G_j \right) \right\rangle_{\mathcal{F}_r}.$$

From these equations, we have

$$\|\hat{\Sigma}_{YX_r}^{(n)} - \Sigma_{YX_r}\|_{\text{HS}}^2 = \|\Sigma_{YX_r}\|_{\text{HS}}^2 - 2\langle \Sigma_{YX_r}, \hat{\Sigma}_{YX_r}^{(n)} \rangle_{\text{HS}} + \|\hat{\Sigma}_{YX_r}^{(n)}\|_{\text{HS}}^2 \quad (9)$$

$$= \left\| \frac{1}{n} \sum_{i=1}^n \left( F_{ri} - \frac{1}{n} \sum_{j=1}^n F_{rj} \right) \left( G_i - \frac{1}{n} \sum_{j=1}^n G_j \right) - \mathbb{E}[F_r G] \right\|_{\mathcal{F}_r}^2 \quad (10)$$

$$= \left\| \frac{1}{n} \sum_{i=1}^n F_{ri} G_i - \mathbb{E}[F_r G] - \left( 2 - \frac{1}{n} \right) \left( \frac{1}{n} \sum_{i=1}^n F_{ri} \right) \left( \frac{1}{n} \sum_{i=1}^n G_i \right) \right\|_{\mathcal{F}_r}^2, \quad (11)$$

which is further bounded by

$$\left\| \frac{1}{n} \sum_{i=1}^n F_{ri} G_i - \mathbb{E}[F_r G] \right\|_{\mathcal{F}_r} + 2 \left\| \left( \frac{1}{n} \sum_{i=1}^n F_{ri} \right) \left( \frac{1}{n} \sum_{i=1}^n G_i \right) \right\|_{\mathcal{F}_r}.$$

Let  $Z_{ri} = F_{ri} G_i - \mathbb{E}[F_r G]$ . Since the variance of a sum of independent random variables is equal to the sum of their variances, we obtain

$$\mathbb{E} \left\| \frac{1}{n} \sum_{i=1}^n Z_{ri} \right\|_{\mathcal{F}_r}^2 = \frac{1}{n} \mathbb{E} \|Z_{r1}\|_{\mathcal{F}_r}^2. \quad (12)$$

$$\begin{aligned} \mathbb{E} \|Z_{r1}\|_{\mathcal{F}_r}^2 &= \mathbb{E} \|F_{r1} G_1 - \mathbb{E}[F_r G]\|_{\mathcal{F}_r}^2 \\ &\leq 2\mathbb{E} \|F_{r1} G_1\|_{\mathcal{F}_r}^2 + 2\|\mathbb{E}[F_r G]\|_{\mathcal{F}_r}^2 \\ &\leq 2\mathbb{E} \|F_{r1}\|_{\mathcal{H}_{X_r}}^2 \|G_1\|_{\mathcal{H}_Y}^2 + 2(\mathbb{E} \|F_r G\|_{\mathcal{F}_r})^2 \\ &\leq 4\mathbb{E} \|F_{r1}\|_{\mathcal{H}_{X_r}}^2 \|G_1\|_{\mathcal{H}_Y}^2 \\ &\leq 64B^2 \end{aligned}$$

The first inequality follows from the fact that  $\|a-b\|^2 \leq 2\|a\|^2 + 2\|b\|^2$ . The second inequality follows from Jensen's inequality  $\|\mathbb{E}[F_r G]\|_{\mathcal{F}_r} \leq \mathbb{E}\|F_r G\|_{\mathcal{F}_r}$ . The third inequality follows from the fact that  $(\mathbb{E}\|F_r G\|_{\mathcal{F}_r})^2 \leq \mathbb{E}\|F_r G\|_{\mathcal{F}_r}^2 \leq \mathbb{E}\|F_r\|_{\mathcal{H}_{X_r}}^2 \|G\|_{\mathcal{H}_Y}^2$ . The last inequality follows from lemma A.3 that  $\|F_{ri}\|_{\mathcal{H}_{X_r}} \leq 2\sqrt{B}$  and  $\|G_i\|_{\mathcal{H}_Y} \leq 2\sqrt{B}$ .

From the inequalities

$$\begin{aligned} \mathbb{E} \left\| \left( \frac{1}{n} \sum_{i=1}^n F_{ri} \right) \left( \frac{1}{n} \sum_{i=1}^n G_i \right) \right\|_{\mathcal{F}_r} &= \mathbb{E} \left[ \left\| \frac{1}{n} \sum_{i=1}^n F_{ri} \right\|_{\mathcal{H}_{X_r}} \left\| \frac{1}{n} \sum_{i=1}^n G_i \right\|_{\mathcal{H}_Y} \right] \\ &\leq \left( \mathbb{E} \left\| \frac{1}{n} \sum_{i=1}^n F_{ri} \right\|_{\mathcal{H}_{X_r}}^2 \right)^{1/2} \left( \mathbb{E} \left\| \frac{1}{n} \sum_{i=1}^n G_i \right\|_{\mathcal{H}_Y}^2 \right)^{1/2}, \end{aligned}$$

and

$$\mathbb{E} \left\| \frac{1}{n} \sum_{i=1}^n F_{ri} \right\|_{\mathcal{H}_{X_r}}^2 = \frac{1}{n} \mathbb{E}\|F_{r1}\|_{\mathcal{H}_{X_r}}^2 \leq \frac{4B}{n},$$

we have

$$\mathbb{E}\|\hat{\Sigma}_{YX_r}^{(n)} - \Sigma_{YX_r}\|_{\text{HS}} \leq (64B^2)^{1/2} n^{-1/2} + 4Bn^{-1} \leq c_1 Bn^{-1/2}$$

for some constant  $c_1 > 0$ . Following the same argument we can show that

$$\mathbb{E}\|\hat{\Sigma}_{X_r X_r}^{(n)} - \Sigma_{X_r X_r}\|_{\text{HS}} \leq c_1 Bn^{-1/2}, \text{ and } \mathbb{E}\|\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY}\|_{\text{HS}} \leq c_1 Bn^{-1/2},$$

To prove part 2, we have by lemma A.2

$$\|\Sigma_{YX_r}\|_{\text{HS}}^2 = \|\mathbb{E}[F_r G]\|_{\mathcal{F}_r}^2 \leq (\mathbb{E}\|F_r\|_{\mathcal{H}_{X_r}} \|G\|_{\mathcal{H}_Y})^2 \leq 16B^2,$$

where the first inequality follows from Jensen's inequality with respect to  $\|\cdot\|_{\mathcal{F}_r}$  and the fact that  $\|F_r G\|_{\mathcal{F}_r} = \|F_r\|_{\mathcal{H}_{X_r}} \|G\|_{\mathcal{H}_Y}$ , and the last inequality follows from lemma A.3.

$$\begin{aligned} \|\hat{\Sigma}_{YX_r}^{(n)}\|_{\text{HS}}^2 &= \left\| \frac{1}{n} \sum_{i=1}^n \left( F_{ri} - \frac{1}{n} \sum_{j=1}^n F_{rj} \right) \left( G_i - \frac{1}{n} \sum_{j=1}^n G_j \right) \right\|_{\mathcal{F}_r}^2 \\ &\leq 2 \left\| \frac{1}{n} \sum_{i=1}^n F_{ri} G_i \right\|_{\mathcal{F}_r}^2 + 2 \left\| \frac{1}{n^2} \sum_{i=1}^n F_{ri} \sum_{i=1}^n G_i \right\|_{\mathcal{F}_r}^2 \\ &\leq 2 \frac{1}{n^2} \sum_{i,j=1}^n \langle F_{ri}, F_{rj} \rangle_{\mathcal{H}_{X_r}} \langle G_i, G_j \rangle_{\mathcal{H}_Y} + 2 \frac{1}{n^4} \sum_{i,j,k,l=1}^n \langle F_{ri}, F_{rj} \rangle_{\mathcal{H}_{X_r}} \langle G_k, G_l \rangle_{\mathcal{H}_Y} \\ &\leq 64B^2, \end{aligned}$$

where the first inequality comes from the fact that  $\|a+b\|^2 \leq 2\|a\|^2 + 2\|b\|^2$  and the last inequality follows from lemma A.3. The proof arguments are similar for  $\Sigma_{X_r X_r}$ ,  $\hat{\Sigma}_{X_r X_r}$ ,  $\Sigma_{YY}$ , and  $\hat{\Sigma}_{YY}$ .  $\square$

**Lemma A.5.** *Let  $\epsilon_n$  be a positive number such that  $\epsilon_n \rightarrow 0 (n \rightarrow \infty)$ . Then, for the i.i.d. sample  $\{(X^{(i)}, Y^{(i)})\}_{i=1}^n$ , we have for  $r = 1, \dots, p$ ,*

$$\mathbb{E} \|\hat{\mathcal{R}}_{YX_r}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\| \leq c_2 K^2 \epsilon_n^{-3/2} n^{-1/2}$$

for some positive constant  $c_2 > 0$ .

*Proof.* Following the same argument as in Fukumizu et al. (2007a), the difference  $\hat{\mathcal{R}}_{YX}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX} (\Sigma_{XX} + \epsilon_n I)^{-1/2}$  can be decomposed as

$$\begin{aligned} & \hat{\mathcal{R}}_{YX}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX} (\Sigma_{XX} + \epsilon_n I)^{-1/2} \\ &= \{(\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-1/2} - (\Sigma_{YY} + \epsilon_n I)^{-1/2}\} \hat{\Sigma}_{YX}^{(n)} (\hat{\Sigma}_{XX}^{(n)} + \epsilon_n I)^{-1/2} \\ & \quad + (\Sigma_{YY} + \epsilon_n I)^{-1/2} \{\hat{\Sigma}_{YX}^{(n)} - \Sigma_{YX}\} (\hat{\Sigma}_{XX}^{(n)} + \epsilon_n I)^{-1/2} \\ & \quad + (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX} \{(\hat{\Sigma}_{XX}^{(n)} + \epsilon_n I)^{-1/2} - (\Sigma_{XX} + \epsilon_n I)^{-1/2}\} \\ &= M_1 + M_2 + M_3 \end{aligned} \tag{13}$$

Using the equality

$$D^{-1/2} - C^{-1/2} = C^{-1/2} (C^{3/2} - D^{3/2}) D^{-3/2} + (D - C) D^{-3/2}, \tag{14}$$

we can rewrite  $M_1$  as

$$\begin{aligned} & \{(\Sigma_{YY} + \epsilon_n I)^{-1/2} ((\Sigma_{YY} + \epsilon_n I)^{3/2} - (\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{3/2}) + (\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY})\} \\ & \quad \times (\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-3/2} \hat{\Sigma}_{YX}^{(n)} (\hat{\Sigma}_{XX}^{(n)} + \epsilon_n I)^{-1/2}, \end{aligned}$$

the norm of which is further upper bounded by

$$\frac{1}{\epsilon_n} \left\{ \frac{3}{\sqrt{\epsilon_n}} \max\{\|\Sigma_{YY} + \epsilon_n I\|^{1/2}, \|\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I\|^{1/2}\} + 1 \right\} \|\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY}\|.$$

The upper bound comes from the fact that  $\|(\Sigma_{YY} + \epsilon_n I)^{-1/2}\| \leq \epsilon_n^{-1/2}$ ,  $(\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-1/2} \hat{\Sigma}_{YX}^{(n)} (\hat{\Sigma}_{XX}^{(n)} + \epsilon_n I)^{-1/2} \leq 1$  (Fukumizu et al., 2007a), and Lemma A.1,

Provided that  $\epsilon_n \rightarrow 0$ , by Lemma A.4 we have

$$\mathbb{E} \|M_1\| \leq c B^{3/2} \epsilon_n^{-3/2} n^{-1/2}$$

for some constant  $c > 0$ . Similarly we have  $\mathbb{E} \|M_3\| \leq c B^{3/2} \epsilon_n^{-3/2} n^{-1/2}$ . From Lemma A.4 and the fact that  $\|(\Sigma_{YY} + \epsilon_n I)^{-1/2}\| \leq \epsilon_n^{-1/2}$ , we know

$$\mathbb{E} \|M_2\| \leq c' \epsilon_n^{-1} n^{-1/2}.$$

So we have for some constant  $c_2 > 0$ ,

$$\mathbb{E} \|\hat{\mathcal{R}}_{YX}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX} (\Sigma_{XX} + \epsilon_n I)^{-1/2}\| \leq c_2 K^{3/2} \epsilon_n^{-3/2} n^{-1/2}.$$

We then complete the proof of the lemma.  $\square$



**Lemma A.6** (McDiarmid's Inequality (McDiarmid (1989))). *Let  $X_1, \dots, X_n$  be independent random variables taking values in a set  $A$ , and assume that  $f; A^n \rightarrow \mathbb{R}$  satisfies*

$$\sup_{x_1, \dots, x_n, x'_i \in A} |f(x_1, \dots, x_n) - f(x_1, \dots, x_{i-1}, x'_i, x_{i+1}, \dots, x_n)| \leq c_i$$

for every  $1 \leq i \leq n$ . Then, for every  $t > 0$ ,

$$\mathbb{P}\{f(X_1, \dots, X_n) - \mathbb{E}f(X_1, \dots, X_n) \geq t\} \leq e^{-2t^2/\sum_{i=1}^n c_i^2}.$$

## A.2 Proof of main theorems

*Proof of Theorem 2.1.* It suffices to check the bounded difference property of  $\|\hat{\Sigma}_{YX_r} - \Sigma_{YX_r}\|_{\text{HS}}$ . Denote  $f((X_r^{(1)}, Y^{(1)}), \dots, (X_r^{(n)}, Y^{(n)})) = \|\hat{\Sigma}_{YX_r}^{(n)} - \Sigma_{YX_r}\|_{\text{HS}}$ . By equation (??)

$$\begin{aligned} \|\hat{\Sigma}_{YX}\|_{\text{HS}} &= \left\| \frac{1}{n} \sum_{i=1}^n \left( F_i - \frac{1}{n} \sum_{j=1}^n F_j \right) \left( G_i - \frac{1}{n} \sum_{j=1}^n G_j \right) \right\|_{\mathcal{F}} \\ &= \left\| \frac{1}{n} \sum_{i=1}^n F_i G_i - \frac{1}{n^2} \sum_{i,j=1}^n F_i G_j \right\|_{\mathcal{F}}, \end{aligned}$$

we have

$$\begin{aligned} &|f((X_r^{(1)}, Y^{(1)}), \dots, (X_r^{(n)}, Y^{(n)})) - f((X_r^{(1)}, Y^{(1)}), \dots, (X_r^{(i)}, Y^{(i)}), \dots, (X_r^{(n)}, Y^{(n)}))| \\ &\leq \|\hat{\Sigma}_{YX_r}^{(n)} - \hat{\Sigma}_{YX_r}^{(n)}\|_{\text{HS}} \\ &= \left\| \frac{1}{n} (F_{ri} G_i - F'_{ri} G'_i) - \frac{1}{n^2} \left\{ \sum_{j \neq i} [(F_{ri} - F'_{ri}) G_j + F_{rj} (G_i - G'_i)] + (F_{ri} G_i - F'_{ri} G'_i) \right\} \right\|_{\mathcal{F}_r} \\ &\leq \left\| \frac{1}{n} (F_{ri} G_i - F'_{ri} G'_i) \right\|_{\mathcal{F}} + \frac{1}{n^2} \left\| \left\{ \sum_{j \neq i} [(F_{ri} - F'_{ri}) G_j + F_{rj} (G_i - G'_i)] + (F_{ri} G_i - F'_{ri} G'_i) \right\} \right\|_{\mathcal{F}_r} \\ &\leq \frac{8B}{n} + \frac{1}{n} (\|(F_{ri} - F'_{ri}) G_1\| + \|F_{r1} (G_i - G'_i)\|) + \frac{8B}{n^2} \\ &\leq \frac{8B}{n} + \frac{8B}{n} + \frac{8B}{n} + \frac{8B}{n^2} \\ &\leq \frac{32B}{n} \end{aligned}$$

The equality follows from the same argument as in proof of Lemma A.2. The second inequality follows from triangle inequality, the third and fourth inequalities follows from Lemma A.3. Then by McDiarmid's inequality we complete the proof.  $\square$

*Proof of Theorem 2.2.* By (13), we have  $\|\hat{\mathcal{R}}_{YX_r}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\| \leq I + II + III$ , where

$$\begin{aligned} I &= \|\{(\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-1/2} - (\Sigma_{YY} + \epsilon_n I)^{-1/2}\} \hat{\Sigma}_{YX_r}^{(n)} (\hat{\Sigma}_{X_r X_r}^{(n)} + \epsilon_n I)^{-1/2}\|, \\ II &= \|(\Sigma_{YY} + \epsilon_n I)^{-1/2} \{\hat{\Sigma}_{YX_r}^{(n)} - \Sigma_{YX_r}\} (\hat{\Sigma}_{X_r X_r}^{(n)} + \epsilon_n I)^{-1/2}\|, \\ III &= \|(\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} \{(\hat{\Sigma}_{X_r X_r}^{(n)} + \epsilon_n I)^{-1/2} - (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\}\|. \end{aligned}$$

By (14) we have

$$I = \|\{(\Sigma_{YY} + \epsilon_n I)^{-1/2}((\Sigma_{YY} + \epsilon_n I)^{3/2} - (\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{3/2}) + (\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY})\} \\ \times (\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-3/2} \hat{\Sigma}_{YX_r}^{(n)} (\hat{\Sigma}_{X_r X_r}^{(n)} + \epsilon_n I)^{-1/2}\|.$$

From  $\|(\Sigma_{YY} + \epsilon_n I)^{-1/2}\| \leq \epsilon_n^{-1/2}$ ,  $\|(\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I)^{-1/2} \hat{\Sigma}_{YX_r}^{(n)} (\hat{\Sigma}_{X_r X_r}^{(n)} + \epsilon_n I)^{-1/2}\| \leq 1$ , and Lemma A.1,

$$I \leq \frac{1}{\epsilon_n} \left\{ \frac{3}{\sqrt{\epsilon_n}} \max\{\|\Sigma_{YY} + \epsilon_n I\|, \|\hat{\Sigma}_{YY}^{(n)} + \epsilon_n I\|\} + 1 \right\} \|\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY}\| \leq cB^{1/2} \epsilon_n^{-3/2} \|\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY}\|_{\text{HS}}$$

By Lemma A.4 and Theorem 2.1, we have

$$\mathbb{P}\{\|\hat{\Sigma}_{YY}^{(n)} - \Sigma_{YY}\|_{\text{HS}} \geq c_1 B n^{-1/2} + t\} \leq \exp(-\frac{nt^2}{512B^2}). \quad (15)$$

Then

$$\mathbb{P}\{I \geq C'_1 B^{3/2} n^{-1/2} \epsilon_n^{-3/2} + cB^{1/2} \epsilon_n^{-3/2} t\} \leq \exp(-\frac{nt^2}{512B^2}). \quad (16)$$

Using a similar argument, we have

$$\mathbb{P}\{III \geq C'_1 B^{3/2} n^{-1/2} \epsilon_n^{-3/2} + cB^{1/2} \epsilon_n^{-3/2} t\} \leq \exp(-\frac{nt^2}{512B^2}). \quad (17)$$

Since  $II \leq \epsilon_n^{-1} \|\hat{\Sigma}_{YX_r}^{(n)} - \Sigma_{YX}\|$ , we have  $\mathbb{P}\{II \geq c_1 B n^{-1/2} \epsilon_n^{-1/2} + \epsilon_n^{-1/2} t\} \leq \exp(-\frac{nt^2}{512B^2})$ . By the condition  $\epsilon_n = o(1)$  we know that

$$\mathbb{P}\{II \geq C'_1 B^{3/2} n^{-1/2} \epsilon_n^{-3/2} + c_3 B^{1/2} \epsilon_n^{-3/2} t\} \leq \exp(-\frac{nt^2}{512B^2}) \quad (18)$$

Let  $t^* = C'_1 B^{3/2} n^{-1/2} \epsilon_n^{-3/2} + c_3 B^{1/2} \epsilon_n^{-3/2} t$ . Then

$$\begin{aligned} & \mathbb{P}\{\|\hat{\mathcal{R}}_{YX_r}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\| \geq 3t^*\} \\ & \leq \mathbb{P}\{I + II + III \geq 3t^*\} \\ & \leq \mathbb{P}\{I \geq t^*\} + \mathbb{P}\{II \geq t^*\} + \mathbb{P}\{III \geq t^*\} \\ & \leq 3 \exp(-\frac{nt^2}{512B^2}) \end{aligned}$$

where the second inequality follows from the union bound. Replace  $3c_3 B^{1/2} \epsilon_n^{-3/2} t$  by  $u$ , we have

$$\begin{aligned} & \mathbb{P}\{\|\hat{\mathcal{R}}_{YX_r}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\| \\ & \quad - C_1 B^{3/2} n^{-1/2} \epsilon_n^{-3/2} \geq u\} \\ & \leq 3 \exp(-\frac{\epsilon_n^3 n u^2}{512B^2}) \end{aligned}$$

where  $C_1 = 3C'_1$ . □

*Proof of Theorem 2.3.* First notice that  $\{|\hat{\rho}_r(\epsilon_n) - \rho_r(\epsilon_n)| \geq cB^{3/2}\epsilon_n^{-3/2}n^{-\kappa}\} \subseteq \{|\hat{\mathcal{R}}_{YX_r}^{(n)} - (\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}| \geq cB^{3/2}\epsilon_n^{-3/2}n^{-\kappa}\}$ . Then by Theorem 2.2 we know for  $0 < \kappa < 1/2$ , there exist  $C_3, C_4 > 0$ , such that

$$\mathbb{P}\{|\hat{\rho}_r(\epsilon_n) - \rho_r(\epsilon_n)| \geq C_3 B^{3/2} \epsilon_n^{-3/2} n^{-\kappa}\} \leq 3 \exp(-C_4 B n^{1-2\kappa})$$

Then by union bound we proved the first part of Theorem 2.3. For the second part, we notice that if  $\mathcal{M} \not\subseteq \hat{\mathcal{M}}$ , then there must exist some  $r \in \mathcal{M}$  such that  $\hat{\rho}_r < C_3 B^{3/2} \epsilon_n^{-3/2} n^{-\kappa}$ . By condition (C2) we know that  $\mathcal{M} \not\subseteq \hat{\mathcal{M}}$  implies  $|\hat{\rho}_r(\epsilon_n) - \rho_r(\epsilon_n)| > C_3 B^{3/2} \epsilon_n^{-3/2} n^{-\kappa}$  for some  $r \in \mathcal{M}$ . So we have

$$\begin{aligned} \mathbb{P}\{\mathcal{M} \subseteq \hat{\mathcal{M}}\} &= 1 - \mathbb{P}\{\mathcal{M} \not\subseteq \hat{\mathcal{M}}\} \\ &\geq 1 - \mathbb{P}\{\max_{r \in \mathcal{M}} |\hat{\rho}_r(\epsilon_n) - \rho_r(\epsilon_n)| > C_3 B^{3/2} \epsilon_n^{-3/2} n^{-\kappa}\} \\ &\geq 1 - 3s \exp(-C_4 B n^{1-2\kappa}) \end{aligned}$$

□

**Lemma A.7.** Suppose  $m_{X_i}$  is the mean element of  $\mathcal{H}_{X_i}$  for  $i = 1, \dots, p$ , and  $\Sigma_{XY}$  is the covariance operator from  $\mathcal{H}_Y$  to  $\mathcal{H}_X$ . Then we have

- (a)  $(m_{X_1}, \dots, m_{X_p})$  is the mean element of  $\mathcal{H}_X$ , denoted by  $m_X$ .
- (b)  $\|\Sigma_{XY}\|_{\text{HS}}^2 = \sum_{i=1}^p \|\Sigma_{X_i Y}\|_{\text{HS}}^2$ .

*Proof.* Assertion (a) follows from, for any  $f = (f_1, \dots, f_p) \in \mathcal{H}_X$ ,

$$\langle f, m_X \rangle_{\mathcal{H}_X} = \sum_{i=1}^p \langle f_i, m_{X_i} \rangle_{\mathcal{H}_{X_i}} = \sum_{i=1}^p \mathbb{E}[f_i(X_i)] = \mathbb{E}\langle f, \kappa_X(\cdot, X) \rangle_{\mathcal{H}_X}.$$

To show (b), by Lemma A.2,

$$\begin{aligned} \|\Sigma_{YX}\|_{\text{HS}}^2 &= \mathbb{E}[\langle k_x(\cdot, X) - m_X, k_x(\cdot, \tilde{X}) - m_X \rangle_{\mathcal{H}_X} \langle k_y(\cdot, Y) - m_Y, k_y(\cdot, \tilde{Y}) - m_Y \rangle_{\mathcal{H}_Y}] \\ &= \mathbb{E}\left[\sum_{i=1}^p \langle k_{x_i}(\cdot, X_i) - m_{X_i}, k_{x_i}(\cdot, \tilde{X}_i) - m_{X_i} \rangle_{\mathcal{H}_{X_i}} \langle k_y(\cdot, Y) - m_Y, k_y(\cdot, \tilde{Y}) - m_Y \rangle_{\mathcal{H}_Y}\right] \\ &= \|\Sigma_{YX_i}\|_{\text{HS}}^2. \end{aligned}$$

□

Note Fukumizu et al. (2007a) showed that  $\Sigma_{XY}$  is Hilbert–Schmidt for any fixed  $p$ . Next, we extend their result to the case where  $p$  grows to infinity.

**Lemma A.8.** Suppose  $\Sigma_{XX}$  is the covariance operator from  $\mathcal{H}_X$  to  $\mathcal{H}_X$ . Then we have

$$\|\Sigma_{YX}\|_{\text{HS}}^2 = O[\lambda_{\max}(\Sigma_{XX})]. \quad (19)$$

*Proof.* First note that  $\|\Sigma_{YX}\|_{\text{HS}}^2$  is bounded by

$$\|\Sigma_{YX}\|_{\text{HS}}^2 \leq \|\Sigma_{XX}^{1/2}\|^2 \cdot \|\Sigma_{YY}^{1/2}\|_{\text{HS}}^2.$$

Then it suffices to show that  $\|\Sigma_{YY}^{1/2}\|_{\text{HS}}^2 = \text{tr}(\Sigma_{YY}) < \infty$ . By definition  $\text{tr}(\Sigma_{YY})$  is equal to

$$\text{tr}(\Sigma_{YY}) = \mathbb{E}[\|\kappa_Y(\cdot, Y) - m_Y\|^2] = \mathbb{E}\kappa_Y(Y, Y) - \|m_Y\|^2,$$

which is finite by Lemma A.3. The proof is completed.  $\square$

*Proof of Theorem 2.4.* By definition,  $\rho_r(\epsilon_n) = \|(\Sigma_{YY} + \epsilon_n I)^{-1/2} \Sigma_{YX_r} (\Sigma_{X_r X_r} + \epsilon_n I)^{-1/2}\| \leq \epsilon_n^{-1} \|\Sigma_{X_r Y}\|$ . Define  $\Sigma_{XY} = (\Sigma_{X_1 Y}, \dots, \Sigma_{X_p Y})$ , then

$$\sum_{r=1}^p \rho_r^2(\epsilon_n) \leq \sum_{r=1}^p \epsilon_n^{-2} \|\Sigma_{X_r Y}\|_{\text{HS}}^2 \leq \epsilon_n^{-2} \|\Sigma_{XY}\|_{\text{HS}}^2 = O(\epsilon_n^{-2} \lambda_{\max}(\Sigma_{XX})) \quad (20)$$

The second last inequality follows from Lemma A.7, and the last equality follows from Lemma A.8. This implies that the number of  $\{r : \rho_r(\epsilon_n) > \eta \epsilon_n^{-1} n^{-\kappa}\}$  cannot exceed  $O(n^{2\kappa} \lambda_{\max}(\Sigma_{XX}))$  for any  $\eta > 0$ , which implies  $|\{r : \rho_r(\epsilon_n) > \eta \epsilon_n^{-3/2} n^{-\kappa}\}| \leq O(n^{2\kappa} \lambda_{\max}(\Sigma_{XX}))$  for any  $\eta > 0$  because  $\epsilon_n \leq 1$ . Thus, on the set

$$B_n = \left\{ \max_{1 \leq r \leq p} |\hat{\rho}_r(\epsilon_n) - \rho_r(\epsilon_n)| \leq \eta \epsilon_n^{-3/2} n^{-\kappa} \right\},$$

the number of  $\{r : \hat{\rho}_r(\epsilon_n) > 2\eta \epsilon_n^{-3/2} n^{-\kappa}\}$  cannot exceed the number of  $\{r : \rho_r(\epsilon_n) > \eta \epsilon_n^{-3/2} n^{-\kappa}\}$ , which is bounded by  $O(n^{2\kappa} \lambda_{\max}(\Sigma_{XX}))$ . By taking  $\eta = C_3/2$ , we have

$$\mathbb{P}\{|\hat{\mathcal{M}} \leq O(n^{2\kappa} \lambda_{\max}(\Sigma_{XX}))|\} \geq \mathbb{P}B_n$$

The conclusion follows from Theorem 2.3.  $\square$

## \*References

1. Shotaro Akaho. A kernel method for canonical correlation analysis. *arXiv preprint cs/0609071*, 2006
2. Nachman Aronszajn. Theory of reproducing kernels. *Transactions of the American mathematical society*, pages 337–404, 1950
3. Francis R Bach and Michael I Jordan. Kernel independent component analysis. *The Journal of Machine Learning Research*, 3:1–48, 2003
4. Charles R Baker. Joint measures and cross-covariance operators. *Transactions of the American Mathematical Society*, 186:273–289, 1973
5. Krishnakumar Balasubramanian, Bharath Sriperumbudur, and Guy Lebanon. Ultrahigh dimensional feature screening via rkhs embeddings. In *Proceedings of the Sixteenth International Conference on Artificial Intelligence and Statistics*, pages 126–134, 2013

6. Emmanuel Candes and Terence Tao. The dantzig selector: statistical estimation when  $p$  is much larger than  $n$ . *The Annals of Statistics*, pages 2313–2351, 2007
7. Jianqing Fan and Runze Li. Variable selection via nonconcave penalized likelihood and its oracle properties. *Journal of the American statistical Association*, 96(456): 1348–1360, 2001
8. Jianqing Fan and Jinchi Lv. Sure independence screening for ultrahigh dimensional feature space. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 70(5):849–911, 2008
9. Jianqing Fan, Richard Samworth, and Yichao Wu. Ultrahigh dimensional feature selection: beyond the linear model. *The Journal of Machine Learning Research*, 10: 2013–2038, 2009
10. Jianqing Fan and Jinchi Lv. A selective overview of variable selection in high dimensional feature space. *Statistica Sinica*, 20(1):101, 2010
11. Jianqing Fan, Yang Feng, and Rui Song. Nonparametric independence screening in sparse ultra-high-dimensional additive models. *Journal of the American Statistical Association*, 106(494), 2011
12. Kenji Fukumizu, Arthur Gretton, Xiaohai Sun, and Bernhard Schölkopf. Kernel measures of conditional dependence. In *NIPS*, volume 20, pages 489–496, 2007b
13. Kenji Fukumizu, Francis R Bach, and Arthur Gretton. Statistical consistency of kernel canonical correlation analysis. *The Journal of Machine Learning Research*, 8:361–383, 2007a
14. Kenji Fukumizu, Francis R Bach, and Michael I Jordan. Kernel dimension reduction in regression. *The Annals of Statistics*, pages 1871–1905, 2009
15. Arthur Gretton, Olivier Bousquet, Alex Smola, and Bernhard Schölkopf. Measuring statistical dependence with hilbert-schmidt norms. In *Algorithmic learning theory*, pages 63–77. Springer, 2005
16. Pengsheng Ji, Jiashun Jin, et al. Ups delivers optimal phase diagram in high-dimensional variable selection. *The Annals of Statistics*, 40(1):73–103, 2012
17. Hyo Jung Kang, Yuka Imamura Kawasaki, Feng Cheng, Ying Zhu, Xuming Xu, Mingfeng Li, André MM Sousa, Mihovil Pletikos, Kyle A Meyer, Goran Sedmak, et al. Spatio-temporal transcriptome of the human brain. *Nature*, 478(7370):483–489, 2011
18. Kuang-Yao Lee, Bing Li, Francesca Chiaromonte, et al. A general theory for nonlinear sufficient dimension reduction: Formulation and estimation. *The Annals of Statistics*, 41(1):221–249, 2013
19. Kuang-Yao Lee, Bing Li, and Hongyu Zhao. Variable selection via additive conditional independence. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 2016

20. Bing Li, Hyonho Chun, and Hongyu Zhao. On an additive semigraphoid model for statistical networks with application to pathway analysis. *Journal of the American Statistical Association*, 109(507):1188–1204, 2014
21. Runze Li, Wei Zhong, and Liping Zhu. Feature screening via distance correlation learning. *Journal of the American Statistical Association*, 107(499):1129–1139, 2012
22. Colin McDiarmid. On the method of bounded differences. *Surveys in combinatorics*, 141(1):148–188, 1989
23. Thomas Melzer, Michael Reiter, and Horst Bischof. Nonlinear feature extraction using generalized canonical correlation analysis. In *Artificial Neural Networks ICANN 2001*, pages 353–360. Springer, 2001
24. Charles A Micchelli, Yuesheng Xu, and Haizhang Zhang. Universal kernels. *The Journal of Machine Learning Research*, 7:2651–2667, 2006
25. Michael Reed and Barry Simon. *Methods of modern mathematical physics: Functional analysis*, volume 1. Gulf Professional Publishing, 1980
26. Dino Sejdinovic, Bharath Sriperumbudur, Arthur Gretton, Kenji Fukumizu, et al. Equivalence of distance-based and rkhs-based statistics in hypothesis testing. *The Annals of Statistics*, 41(5):2263–2291, 2013
27. Le Song, Alex Smola, Arthur Gretton, Justin Bedo, and Karsten Borgwardt. Feature selection via dependence maximization. *The Journal of Machine Learning Research*, 13(1):1393–1434, 2012
28. Robert Tibshirani. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 267–288, 1996
29. A Jeremy Willsey, Stephan J Sanders, Mingfeng Li, Shan Dong, Andrew T Tebbenkamp, Rebecca A Muhle, Steven K Reilly, Leon Lin, Sofia Fertuzinhos, Jeremy A Miller, et al. Coexpression networks implicate human midfetal deep cortical projection neurons in the pathogenesis of autism. *Cell*, 155(5):997–1007, 2013
30. Yoshihiro Yamanishi, J-P Vert, Akihiro Nakaya, and Minoru Kanehisa. Extraction of correlated gene clusters from multiple genomic data by generalized kernel canonical correlation analysis. *Bioinformatics*, 19(suppl 1):i323–i330, 2003
31. Cun-Hui Zhang. Nearly unbiased variable selection under minimax concave penalty. *The Annals of Statistics*, pages 894–942, 2010
32. Peng Zhao and Bin Yu. On model selection consistency of lasso. *The Journal of Machine Learning Research*, 7:2541–2563, 2006
33. Hongkui Zeng, Elaine H Shen, John G Hohmann, Seung Wook Oh, Amy Bernard, Joshua J Royall, Katie J Glattfelder, Susan M Sunkin, John A Morris, Angela L Guillozet-Bongaarts, et al. Large-scale cellular-resolution gene profiling in human neocortex reveals species-specific molecular signatures. *Cell*, 149(2):483–496, 2012